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Compressible Multiphase Flows in an ALE Framework

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Compressible Multiphase Flows in An ALE Framework

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Requirements of the Multiphase Flow Model

- The ability to transition from compressible to incompressible regimes (high to low Mach numbers).
 - The ability to generate and simulate distributions of particles or droplets
 - An accurate ALE (Arbitrary Lagrangian/Eulerian) capability for dynamically changing computational domains.
1. Engine cylinders and nozzles
 2. Ablation processes.



Eulerian Multiphase Simulation in ALE3D

- High particle number concentrations often preclude the use of stochastic particle techniques.
- The continuum two-phase model of Baer and Nunziato (SNL) with modifications form the basis of the ALE3D implementation.
- Averaged equations for mass, momentum, and energy are integrated for each phase.
- The ALE methodology is preserved enabling the Lagrangian/Eulerian simulation of dynamically changing computational domains.

Eulerian multiphase models suffer from all the deficiencies of SGS modeling and more.



- **Unresolved fluid motions require parameterization.**
- **Particle/fluid and particle/particle interactions are also parameterized**
 1. **Drag**
 2. **Compaction.**
 3. **Pressure work.**
 4. **Particle spin and other particle/fluid interactions. (BBO Equation terms).**
 5. **Conduction.**



The Multiphase Equations (2-phase)

$$\frac{\partial}{\partial t} \phi_s + \vec{u}_s \cdot \nabla \phi_s = 0$$

$$\frac{\partial}{\partial t} \overline{\rho}_s + \nabla \cdot \overline{\rho}_s \vec{u}_s = \dot{m}$$

$$\frac{\partial}{\partial t} \overline{\rho}_s u_{sj} + \nabla \cdot \overline{\rho} u_s u_{sj} + \frac{\partial}{\partial x_j} \phi_s P_s = \dot{m} V_i + P_i \frac{\partial}{\partial x_j} \phi_s + F_d$$

$$\frac{\partial}{\partial t} \overline{\rho}_s E_s + \nabla \cdot \overline{\rho} u_s E_s + \nabla \cdot \phi_s \vec{u}_s P_s = \dot{m} E_i + P_i V_i \cdot \nabla \phi_s + F_d V_i + Q$$

$$\frac{\partial}{\partial t} \overline{\rho}_g + \nabla \cdot \overline{\rho}_g \vec{u}_g = -\dot{m}$$

$$\frac{\partial}{\partial t} \overline{\rho}_g u_{gj} + \nabla \cdot \overline{\rho} u_g u_{gj} + \frac{\partial}{\partial x_j} \phi_g P_g = -\dot{m} V_i - P_i \frac{\partial}{\partial x_j} \phi_s - F_d$$

$$\frac{\partial}{\partial t} \overline{\rho}_g E_g + \nabla \cdot \overline{\rho} u_g E_g + \nabla \cdot \phi_g \vec{u}_g P_g = -\dot{m} E_i - P_i V_i \cdot \nabla \phi_s - F_d V_i - Q$$

transport = non – conservative terms

■ Various published forms arise depending on the parameterization of the interfacial velocity, pressure, and energy.

ϕ_s = solid volume fraction

$\overline{\rho}_s$ = solid bulk density ($\phi_s \rho_s$)

\dot{m} = solid to gas source term

V_i = interfacial velocity

P_i = interfacial pressure

E_i = interfacial energy

F_d = drag on the gas

Q = heat conduction from gas

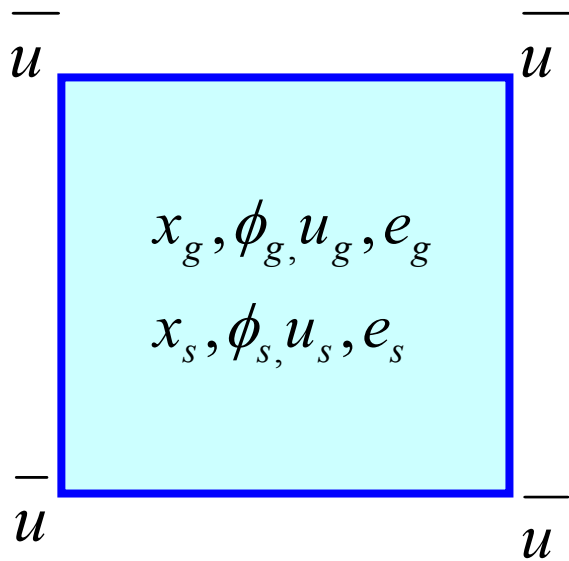


Introduction to ALE methods

- **ALE methods combine Lagrangian methods that are highly accurate for solid mechanics applications with Eulerian advection for a mesh for robustness.**
- 1. Nodes are Lagrangianly moved according to $F=ma$.**
- 2. Internal energy and material properties are integrated due to the change in element size/shape.**
- 3. Properties are advected to a “relaxed” mesh to avoid problems with mesh tangling, distorted elements, etc.**



The Current Ale Multiphase Algorithm



$$\overline{u} = x_g u_g + x_s u_s$$

1. Integrate the bulk Nodal velocities and determine new nodal positions
2. Compute multiphase source terms
3. Integrate phase velocities
4. Integrate phase thermodynamic data
5. Compute multiphase drift
6. Compute Advection.



Verification of the Multiphase Model

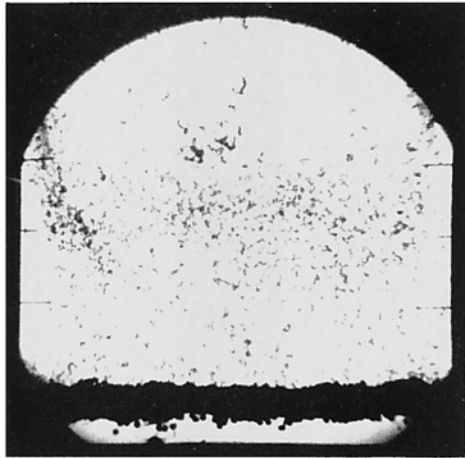
- Several test cases have been identified.
 1. Analytic solutions as unit tests of individual routines
 2. A fluidized bed of glass beads. The bed is fluidized by a Mach 1.3 shock.
 3. A spherical dispersal of solid particles.



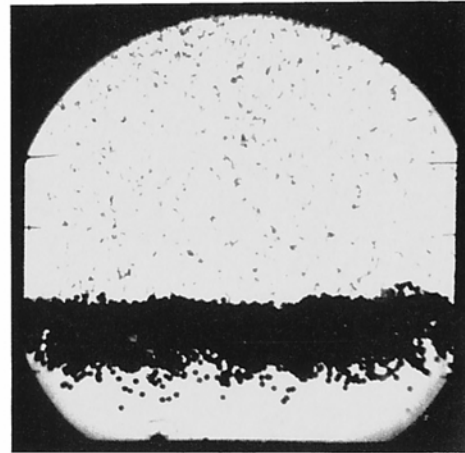
Comparison with Analytic Solutions

- Analytic solutions for the Baer and Nunziato system exist: Nikolai Andrianov and Gerald Warnacke, “The Riemann problem for the Baer-Nunziato two-phase flow model”, *J. Comp. Phys.*, (2004) in press.
- Saurell and Abigail (*J. Comp. Phys.*, 1999) present several test problems with analytic solutions.
- These analytic problems are very useful unit tests.

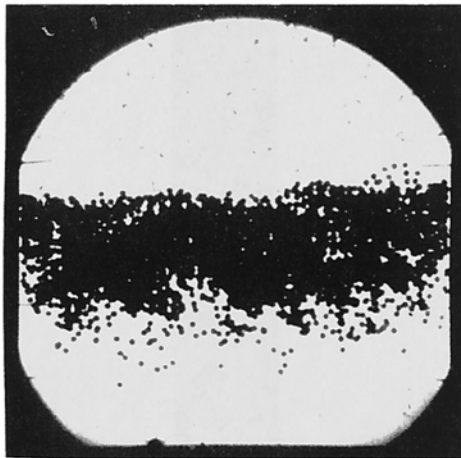
Shock Tube Validation



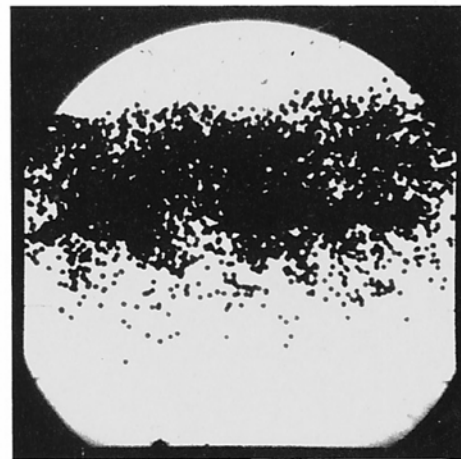
$t = 0.00150 \text{ s}$



$t = 0.00228 \text{ s}$



$t = 0.00318 \text{ s}$



$t = 0.00384 \text{ s}$

■ At left is Figure 11 from Rogue, Rodriguez, Haas, and Saurel's: "Experimental and numerical investigation of the shock-induced fluidization of a particle bed, *Shock Waves*, **8**, 29-45, 1998.

■ This is a series of shadowgraphs of a 2 mm bed of nylon beads being accelerated by a Ma 1.3 shock. Each panel represents a different time in the experiment..

Shock Tube Validation

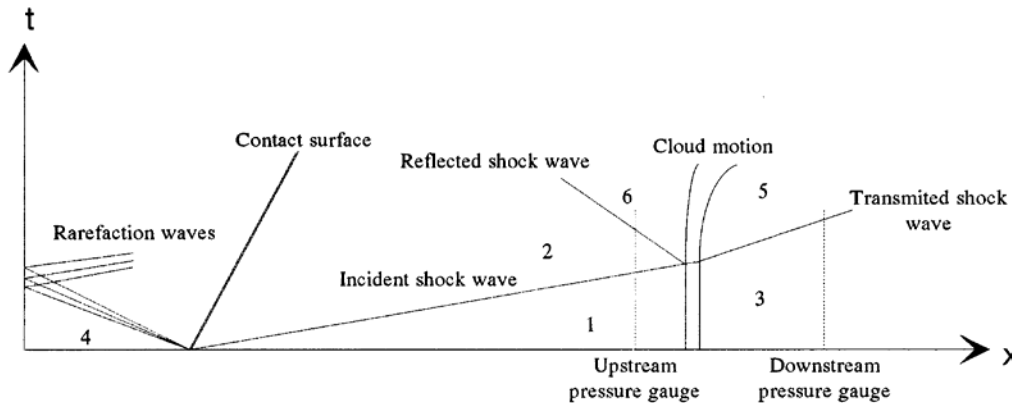
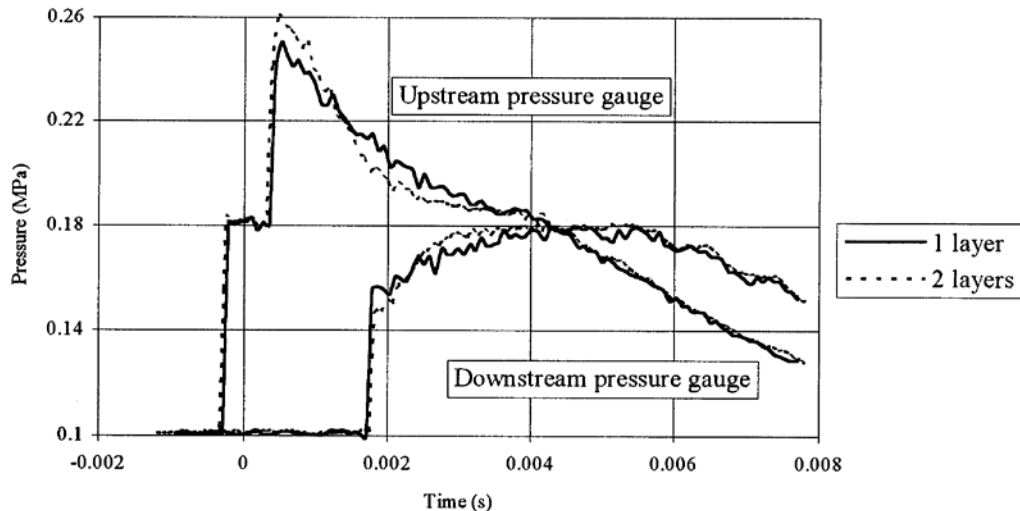


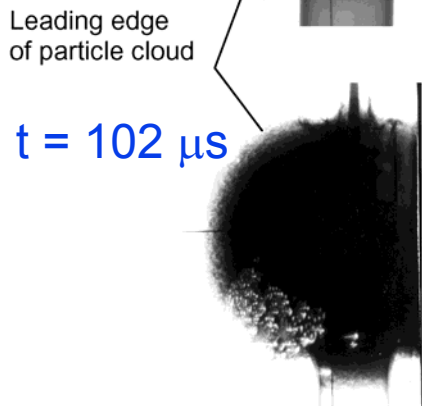
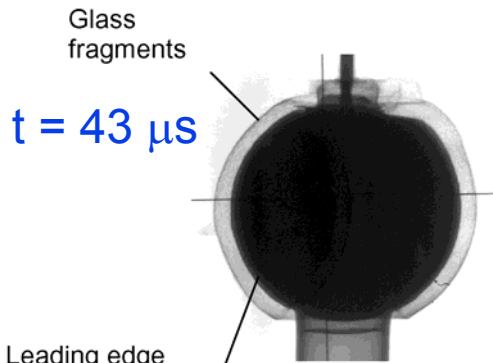
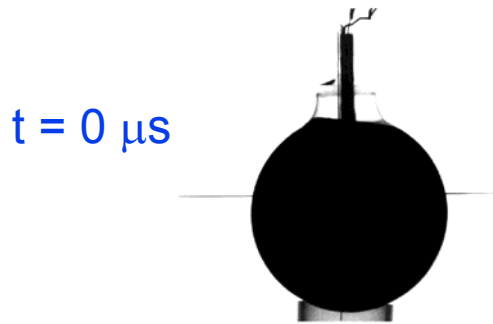
Fig. 15. Schematic (x-t) diagram of the two-phase flow in the shock tube



■ At left are Figures 15-16 from Rogue, Rodriguez, Haas, and Saurel's: "Experimental and numerical investigation of the shock-induced fluidization of a particle bed, *Shock Waves*, **8**, 29-45, 1998.

■ Validation objective is to reproduce the signatures seen at the two pressure gauges.

Multidimensional Validation of the multiphase model.



- At left is Figure 2 from Fan Zhang et al.'s: "Explosive dispersal of solid particles, *Shock Waves*, **10**, 431-443, 2001.
- This is a series of x-ray radiographs of an energetic dispersal of spherical particles. Each panel represents a different time in the experiment.
- This dataset contains several multiphase phenomena for model validation.

Effect of Particle Size on Dispersion

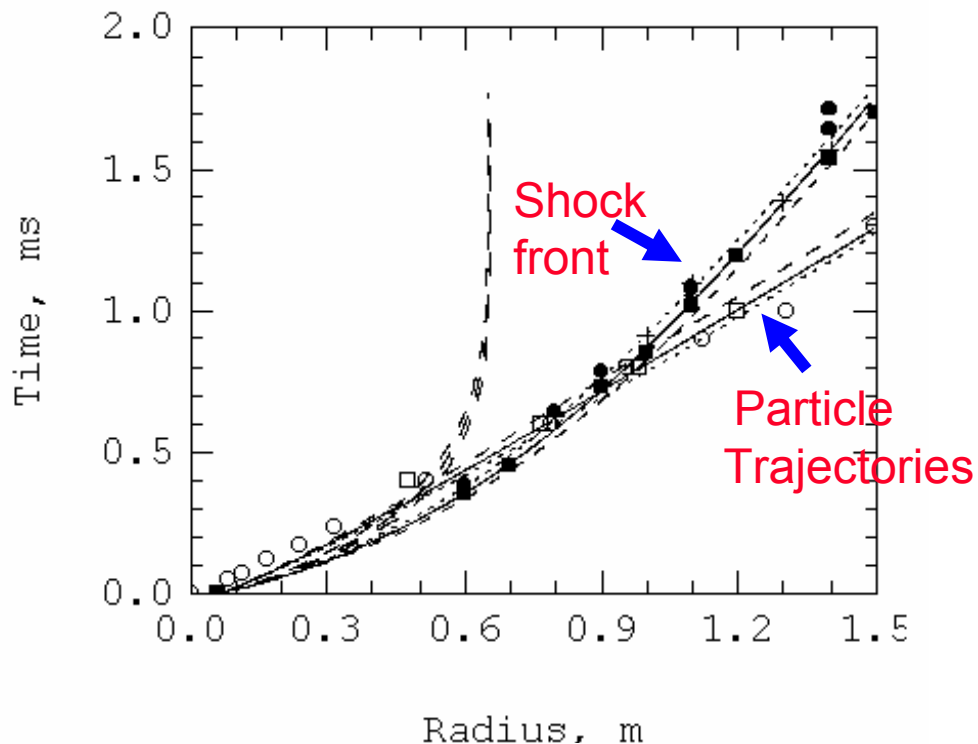


Figure 11 from Fan Zhang et al.

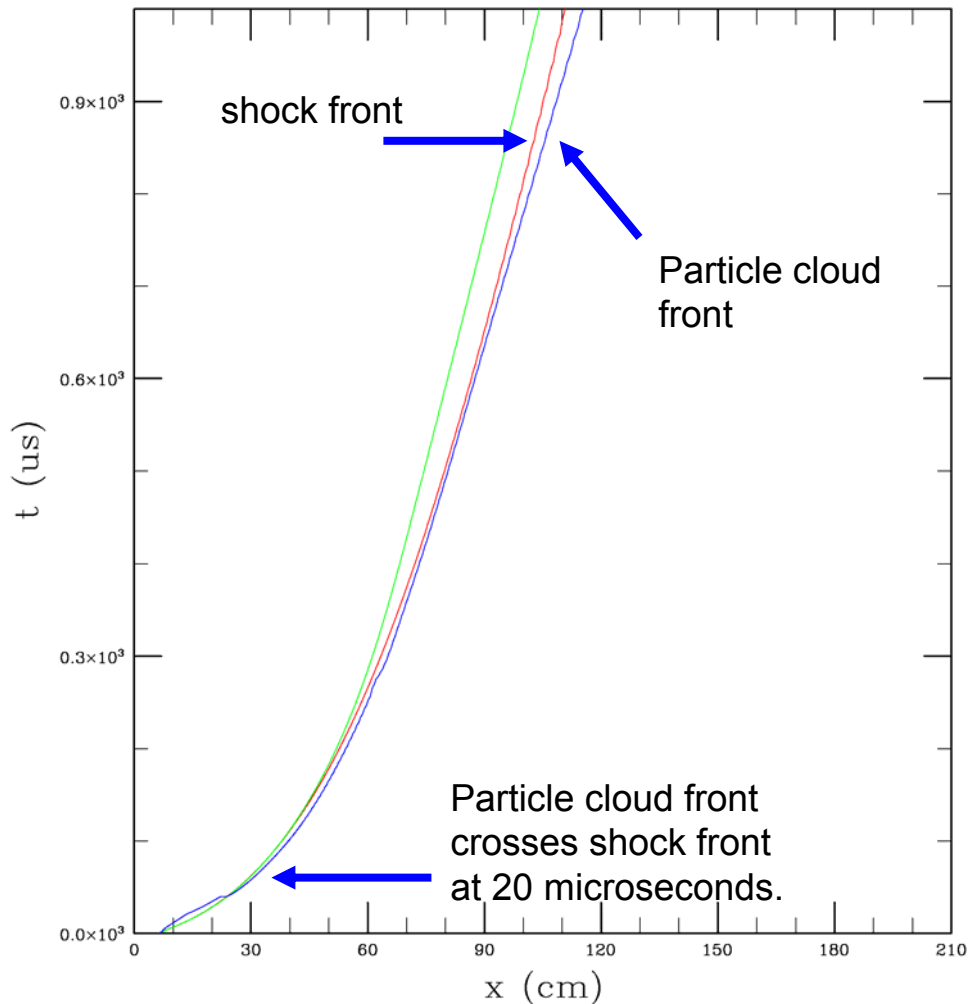
- Particle Size is a very important component of the dispersion in this experiment.
- Large particles (hollow symbols) are able to penetrate the shock front at large times. Smaller particles (not shown) are entrained into the shock front.
- The experimental location of the shock front is denoted by the solid symbols.
- The solid lines are the results of Fan Zhang's Eulerian multiphase model.



Current Progress

- **Current development has iterated between a 1D spherical python model and ALE3D.**
- **The 1D model has resulted in a compressed prototyping/testing cycle in ALE3D.**
- **We have performed initial simulations for eventual comparison with the Fan Zhang data.**
- **The ALE3D implementation has greatly influenced ALE3D's numerical advection and motivated other improvements.**

Preliminary Multiphase Results.



- initial charge diameter of 6 centimeters.

- 1D radial mesh with 0.25 cm zoning in the charge, geometrically expanding to 3 cm at 2 meter radius.

- Lack of separation between particle cloud front and the shock front is probably due to the simple drag model.



Connection Between ALE and Riemann Methods

- Riemann methods have been recently extended to multiphase flows.
- The methods are SGS in spirit in that they encode at the grid level, the non-linear behavior of the PDE.
- These methods use characteristic variables to minimize numerical error and the need for artificial dissipation.
- ALE solvers are also characteristic methods, but use simpler notions about leading order effects.
- Techniques from Riemann methods are improving the ALE3D multiphase model via a “multiphase” monotonic Q.



A New Monotonic Q

$$\rho \frac{Dv}{Dt} = -\frac{\partial}{\partial r} (p + q) r^2$$

$$\frac{1}{\rho} \frac{D\rho}{Dt} = -\frac{1}{r^2} \frac{\partial v r^2}{\partial r}$$

$$\rho \frac{De}{Dt} = -(p + q) \frac{\partial v r^2}{\partial r}$$

Spherical Euler equations for mass, momentum, and internal energy for a single component fluid.

- Lagrangian models make direct use of the material time derivative.
- For stability, explicit models make use of an artificial viscosity, q , in regions of compression (shocks).
- The current ALE3D monotonic q uses a Van Leer slope limiter to minimize its application in non-shocked regions of the flow.
- For a single component fluid, the monotonic q is equivalent to the leading order solution for a Riemann solver.
- We are extending this technique to multiphase flows.



Long Time Scale Evolution

- Many multiphase problems transition from high to low mach numbers.
- Through pressure equilibration techniques taken from the KIVA model developed at LANL, the ALE3D multiphase model will be able to simulate beyond the current millisecond limit to that of seconds.
- This requires the use of advanced Poisson solvers such as those produced by the HYPRE project (LLNL).



Pressure Equilibration

$$P_{eq} = P_i + \left. \frac{\partial P_i}{\partial V_i} \right|_S DV_i$$

$$P_{eq} = \bar{P} + \left. \frac{\partial P}{\partial V} \right|_S DV$$

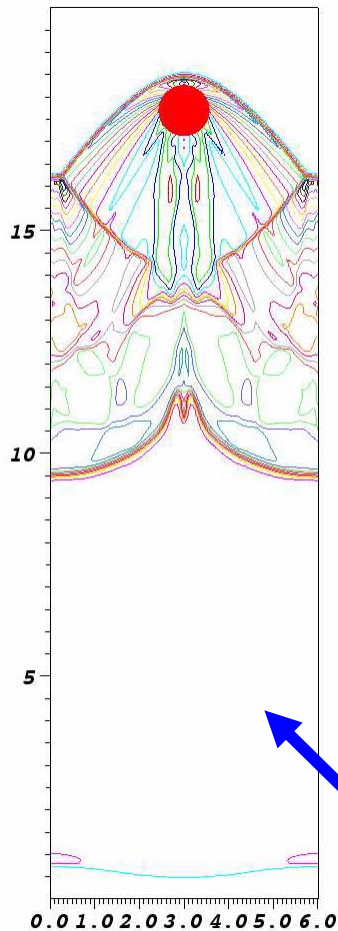
$$RHS = d\hat{P} + \left(\left. \frac{\partial P}{\partial V} \right|_S \right) \left(\frac{M \Delta t^2 \Phi_p}{\rho_o} \right) \sum_{faces} \frac{\nabla_a d\hat{P}}{M_a}$$

- The individual pressure responses relax to an equilibrium pressure

- This equilibrium pressure can be found by solving for an initial bulk pressure and bulk modulus

- After some manipulation and defining zonal gradients, one can define a non-linear outer iteration containing a Poisson problem for an update to the bulk pressure.

Direct Numerical Simulation (DNS)



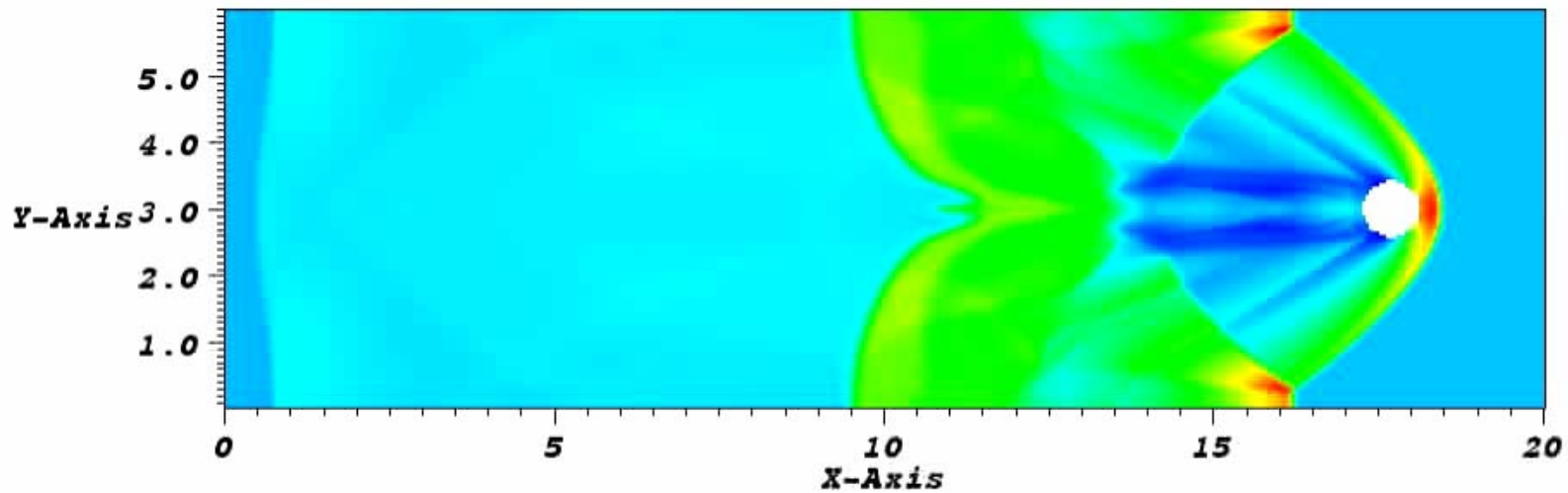
- Direct numerical simulation of particles passing through a shock front is being carried out by the UCSB developed MuSiC simulation system.

- Particles in these simulations are represented via level-sets embedded in a logically rectangular mesh.

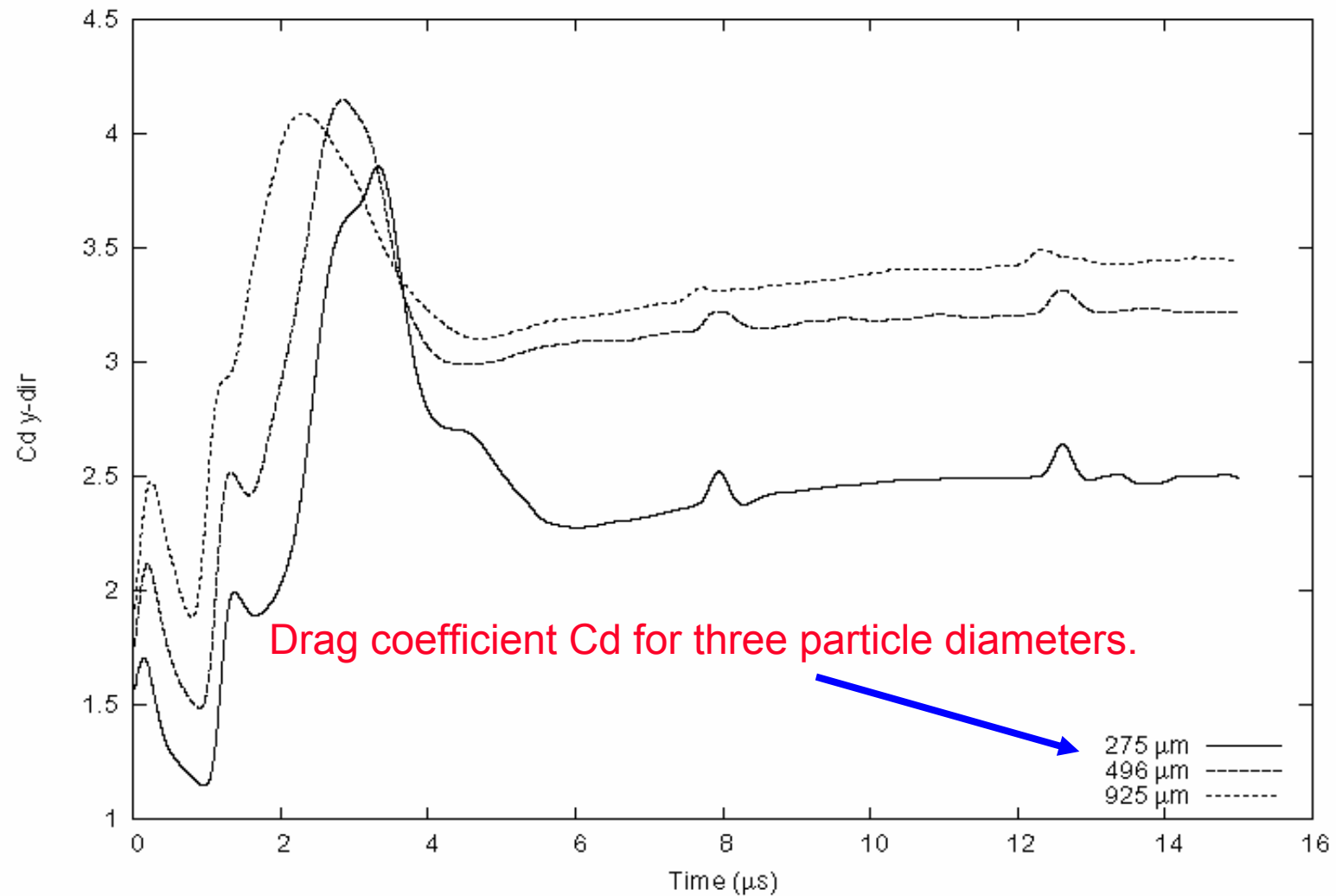
- This level set approach enables the study of particle interaction and deformation in a manner that conformal meshes are unable to reproduce.

Level-set simulation of a particle (RED) in a 6x20 millimeter domain overtaking and passing through a shock after 15 μ s of simulation. The shock is located at 10 millimeters.

Level Set Evolution

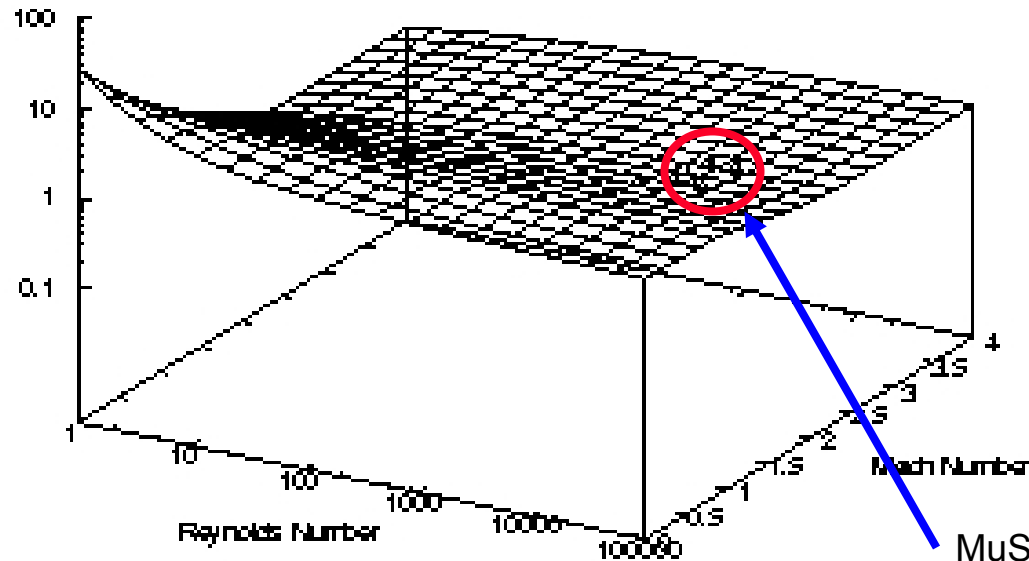


DNS Produced Drag Coefficient





MuSiC results agree with prior empirical drag laws



MuSiC results lie close to the Drag coefficients given by Henderson (1976) derived for particulate flow in rocket engines.



Scaling the microscale to the macroscale

$$m_p \frac{Dv}{Dt} = \frac{\rho_g C_d A_p}{2} |u - v| (u - v)$$

$$\overline{\rho_p} \frac{Dv}{Dt} = \frac{\overline{\rho_p}}{\tau_v} (u - v)$$

$$\tau_v = \frac{4D_p \rho_p}{3\rho_g C_d |u - v|}$$

■ Given a drag coefficient C_d , the particle momentum equation can be summed over all particles to yield an averaged drag force.

■ This drag force can be expressed as being inversely proportional to a velocity relaxation time scale t_v .

■ This time scale is a function of the particle diameter D , the particle and gas densities, and the difference between the gas and fluid velocities $|u-v|$.



Summary

- **Experimental validation datasets have been identified.**
- **ALE methods are being extended with theory taken from established Riemann solvers.**
- **The ALE method is being extended to simulate long timescales.**
- **The results from this project are poised to make a strong impact.**

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